ELSEVIER

Chemical Physics 230 (1998) 347–349

Chemical Physics

Author index to volume 230

Abe, S., see Kato, T. 230 (1998) 209
Andrews, L., see Galland, N. 230 (1998) 143
Azumi, T., see Iwasaki, Y. 230 (1998) 201

Berthier, G., see Daoudi, A. 230 (1998) 31
Bougeard, D., see Smirnov, K.S. 230 (1998) 57
Brenn, R., see Lange, M. 230 (1998) 117
Brereton, G.J., R.J. Crilly and J.R. Spears, Nucleation in small capillary tubes 230 (1998) 253
Brion, C.E., see Rolke, J. 230 (1998) 153
Burda, J.V., A quantum chemical ab initio study of the interaction between Co^+ and Ni^+ ions with CO_2 and N_2O 230 (1998) 13

Chen, C., F. Wang, Y. Chen and X. Ma, Temperature effect on quenching of $CH(A^2\Delta)$ 230 (1998) 317
Chen, Y., see Chen, C. 230 (1998) 317
Ciesielski, K., see Goworek, T. 230 (1998) 305
Crilly, R.J., see Brereton, G.J. 230 (1998) 253

Daoudi, A., S. Elkhattabi, G. Berthier and J.P. Flament, On the electronic structure and spectroscopy of the ScN molecule 230 (1998) 31
Davidson, E.R., see Rolke, J. 230 (1998) 153

Ehara, M., see Hasegawa, J. 230 (1998) 23
Elkhattabi, S., see Daoudi, A. 230 (1998) 31
Ermoshin, V.A., see Smirnov, K.S. 230 (1998) 57

Ferrari, C., see Tombari, E. 230 (1998) 267
Flament, J.P., see Daoudi, A. 230 (1998) 31

Galland, N., Y. Hannachi, D.V. Lanzisera and L. Andrews, Theoretical study of structures, energetics and vibrational properties of BC_2H_3 species 230 (1998) 143
Girardet, C., J. Humbert and P.N.M. Hoang, Theoretical approach of the infrared profile of molecular adsorbates on clean surfaces: inhomogeneous broadening 230 (1998) 67
Goworek, T., K. Ciesielski, B. Jasińska and J. Wawryszczuk, Positronium states in the pores of silica gel 230 (1998) 305

Hannachi, Y., see Galland, N. 230 (1998) 143
Hasegawa, J., M. Ehara and H. Nakatsuji, Theoretical study on the ionized states of ethylene by the SAC-CI (general-*R*) method 230 (1998) 23
Hayes, M.A., see Shaw, D.A. 230 (1998) 97
Hoang, P.N.M., see Girardet, C. 230 (1998) 67

PII S0301-0104(98)00148-7

Holland, D.M.P., see Shaw, D.A. 230 (1998) 97
Holmlid, L., Nanosecond switching, field reversal evidence of Rydberg atom desorption from surfaces 230 (1998) 327
Humbert, J., see Girardet, C. 230 (1998) 67

Iwasaki, Y., H. Murai, K. Maeda and T. Azumi, Study on the coherent spin motion of the radical-ion pair formed in the laser photolysis of *N,N,N′,N′*-tetramethyl-1,4-phenylenediamine in 2-propanol 230 (1998) 201
Iwata, S., see Zhan, C.-G. 230 (1998) 45

Jang, S., M. Zhao and S.A. Rice, Semiclassical quantum unimolecular reaction rate theory revisited 230 (1998) 237
Jasińska, B., see Goworek, T. 230 (1998) 305
Johari, G.P., see Tombari, E. 230 (1998) 267
Johnson, C.A.F., see Shaw, D.A. 230 (1998) 97

Kato, T., F. Sasaki, S. Abe and S. Kobayashi, Theoretical study on the absorption spectra of pseudoisocyanine bromide (PIC-Br) molecular *J*-aggregates 230 (1998) 209
Kobayashi, S., see Kato, T. 230 (1998) 209
Krawczyk, S., Absorption and electroabsorption spectra of carotenoid cation radical and dication 230 (1998) 297
Krimm, S., see Lee, S.-H. 230 (1998) 277

Laenen, R. and C. Rauscher, Numerical study of induced polarization dynamics in ultrafast spectral hole-burning experiments 230 (1998) 223
Lange, M., O. Pfaff, U. Müller and R. Brenn, Projectile fragment–ion fragment–ion coincidences (PFIFICO) following fast ion impact on SF_6 230 (1998) 117
Lanzisera, D.V., see Galland, N. 230 (1998) 143
Lee, S.-H. and S. Krimm, General treatment of vibrations of helical molecules and application to transition dipole coupling in amide I and amide II modes of α-helical poly(L-alanine) 230 (1998) 277

Ma, X., see Chen, C. 230 (1998) 317
MacDonald, M.A., see Shaw, D.A. 230 (1998) 97
Maeda, K., see Iwasaki, Y. 230 (1998) 201
Mishra, P.C., see Shukla, M.K. 230 (1998) 187
Müller, U., see Lange, M. 230 (1998) 117
Murai, H., see Iwasaki, Y. 230 (1998) 201

Nakatsuji, H., see Hasegawa, J. 230 (1998) 23
Naumkin, F.Y., Erratum to "Single- versus multi-state DIM model for Rg X_2 systems: On the influence of spin–orbit coupling on Ar–I_2 potentials" [Chem. Phys. 226 (1998) 319–335] 230 (1998) 345
Nguyen, M.T., R. Sumathi, D. Sengupta and J. Peeters, Theoretical analysis of reactions related to the HNO_2 energy surface: OH + NO and H + NO_2 230 (1998) 1

Parker, J.E., see Shaw, D.A. 230 (1998) 97
Peeters, J., see Nguyen, M.T. 230 (1998) 1
Penzkofer, A., see Reindl, S. 230 (1998) 83
Pfaff, O., see Lange, M. 230 (1998) 117

Rauscher, C., see Laenen, R. 230 (1998) 223
Reindl, S. and A. Penzkofer, Higher excited-state photoisomerization and singlet to triplet intersystem-crossing in DODCI 230 (1998) 83
Rennie, E.E., see Shaw, D.A. 230 (1998) 97
Rice, S.A., see Jang, S. 230 (1998) 237
Rolke, J., Y. Zheng, C.E. Brion, Y.A. Wang and E.R. Davidson, Valence orbital electron momentum distributions for oxygen: comparison of EMS measurements with theory 230 (1998) 153

Salvetti, G., see Tombari, E. 230 (1998) 267
Sasaki, F., see Kato, T. 230 (1998) 209
Sengupta, D., see Nguyen, M.T. 230 (1998) 1
Shaw, D.A., D.M.P. Holland, M.A. MacDonald, M.A. Hayes, L.G. Shpinkova, E.E. Rennie, C.A.F. Johnson, J.E. Parker and W. von Niessen, An experimental and theoretical study of the spectroscopic and thermodynamic properties of toluene 230 (1998) 97
Shpinkova, L.G., see Shaw, D.A. 230 (1998) 97
Shukla, M.K. and P.C. Mishra, An ab initio study of electronic spectra and excited-state properties of 7-azaindole in vapour phase and aqueous solution 230 (1998) 187
Smirnov, K.S., V.A. Ermoshin and D. Bougeard, A classical molecular dynamics study of the vibrational dynamics of the H/C(111)-(1 × 1) system 230 (1998) 57
Spears, J.R., see Brereton, G.J. 230 (1998) 253
Sumathi, R., see Nguyen, M.T. 230 (1998) 1

Tombari, E., C. Ferrari, G. Salvetti and G.P. Johari, Dynamic heat capacity and reaction enthalpy during the two-stage network growth in diepoxide–diamine compositions 230 (1998) 267

Von Niessen, W., see Shaw, D.A. 230 (1998) 97

Wang, F., see Chen, C. 230 (1998) 317
Wang, Y.A., see Rolke, J. 230 (1998) 153
Wawryszczuk, J., see Goworek, T. 230 (1998) 305

Zhan, C.-G. and S. Iwata, Ab initio MO and density functional studies on the vibrational spectra of 1,4-benzoquinone, and its anion and dianion 230 (1998) 45
Zhao, M., see Jang, S. 230 (1998) 237
Zheng, Y., see Rolke, J. 230 (1998) 153

ELSEVIER

Chemical Physics 351–358

Chemical Physics

Subject index to volume 230

Methods and constructs

Theoretical

Computational methods for electronic structure

Theoretical analysis of reactions related to the HNO_2 energy surface: OH + NO and H + NO_2, M.T. Nguyen, R. Sumathi, D. Sengupta and J. Peeters 230 (1998) 1

A quantum chemical ab initio study of the interaction between Co^+ and Ni^+ ions with CO_2 and N_2O, J.V. Burda 230 (1998) 13

Theoretical study on the ionized states of ethylene by the SAC-CI (general-*R*) method, J. Hasegawa, M. Ehara and H. Nakatsuji 230 (1998) 23

-CI and valence bond approach

On the electronic structure and spectroscopy of the ScN molecule, A. Daoudi, S. Elkhattabi, G. Berthier and J.P. Flament 230 (1998) 31

Theoretical study of structures, energetics and vibrational properties of BC_2H_3 species, N. Galland, Y. Hannachi, D.V. Lanzisera and L. Andrews 230 (1998) 143

Valence orbital electron momentum distributions for oxygen: comparison of EMS measurements with theory, J. Rolke, Y. Zheng, C.E. Brion, Y.A. Wang and E.R. Davidson 230 (1998) 153

An ab initio study of electronic spectra and excited-state properties of 7-azaindole in vapour phase and aqueous solution, M.K. Shukla and P.C. Mishra 230 (1998) 187

-perturbative and many body approaches

Ab initio MO and density functional studies on the vibrational spectra of 1,4-benzoquinone, and its anion and dianion, C.-G. Zhan and S. Iwata 230 (1998) 45

-density functional theory

Ab initio MO and density functional studies on the vibrational spectra of 1,4-benzoquinone, and its anion and dianion, C.-G. Zhan and S. Iwata 230 (1998) 45

Theoretical study of structures, energetics and vibrational properties of BC_2H_3 species, N. Galland, Y. Hannachi, D.V. Lanzisera and L. Andrews 230 (1998) 143

Valence orbital electron momentum distributions for oxygen: comparison of EMS measurements with theory, J. Rolke, Y. Zheng, C.E. Brion, Y.A. Wang and E.R. Davidson 230 (1998) 153

Wavefunctions for highly excited and unbound states

Theoretical study on the ionized states of ethylene by the SAC-CI (general-*R*) method, J. Hasegawa, M. Ehara and H. Nakatsuji 230 (1998) 23

Spin states and magnetic interactions
Study on the coherent spin motion of the radical-ion pair formed in the laser photolysis of *N,N,N′,N′*-tetramethyl-1,4-phenylenediamine in 2-propanol, Y. Iwasaki, H. Murai, K. Maeda and T. Azumi 230 (1998) 201

Molecular response to external fields (incl. optical susceptibilities, dichroism, hyperpolarizabilities)
Theoretical study on the absorption spectra of pseudoisocyanine bromide (PIC-Br) molecular *J*-aggregates, T. Kato, F. Sasaki, S. Abe and S. Kobayashi 230 (1998) 209
Numerical study of induced polarization dynamics in ultrafast spectral hole-burning experiments, R. Laenen and C. Rauscher 230 (1998) 223

Intramolecular dynamics
Semiclassical quantum unimolecular reaction rate theory revisited, S. Jang, M. Zhao and S.A. Rice 230 (1998) 237
General treatment of vibrations of helical molecules and application to transition dipole coupling in amide I and amide II modes of α-helical poly(L-alanine), S.-H. Lee and S. Krimm 230 (1998) 277

Molecular dynamics of many particle systems and condensed phases
A classical molecular dynamics study of the vibrational dynamics of the H/C(111)-(1 × 1) system, K.S. Smirnov, V.A. Ermoshin and D. Bougeard 230 (1998) 57
Theoretical approach of the infrared profile of molecular adsorbates on clean surfaces: inhomogeneous broadening, C. Girardet, J. Humbert and P.N.M. Hoang 230 (1998) 67

Non-equilibrium thermodynamic and hydrodynamic theories
Nucleation in small capillary tubes, G.J. Brereton, R.J. Crilly and J.R. Spears 230 (1998) 253

Equilibrium statistical mechanics and thermodynamics
Dynamic heat capacity and reaction enthalpy during the two-stage network growth in diepoxide–diamine compositions, E. Tombari, C. Ferrari, G. Salvetti and G.P. Johari 230 (1998) 267

Experiment

Magnetic resonances
Study on the coherent spin motion of the radical-ion pair formed in the laser photolysis of *N,N,N′,N′*-tetramethyl-1,4-phenylenediamine in 2-propanol, Y. Iwasaki, H. Murai, K. Maeda and T. Azumi 230 (1998) 201

-Molecular spectroscopy
An ab initio study of electronic spectra and excited-state properties of 7-azaindole in vapour phase and aqueous solution, M.K. Shukla and P.C. Mishra 230 (1998) 187
Theoretical study on the absorption spectra of pseudoisocyanine bromide (PIC-Br) molecular *J*-aggregates, T. Kato, F. Sasaki, S. Abe and S. Kobayashi 230 (1998) 209

-infrared
Theoretical approach of the infrared profile of molecular adsorbates on clean surfaces: inhomogeneous broadening, C. Girardet, J. Humbert and P.N.M. Hoang 230 (1998) 67

General treatment of vibrations of helical molecules and application to transition dipole coupling in amide I and amide II modes of α-helical poly(L-alanine), S.-H. Lee and S. Krimm 230 (1998) 277
Absorption and electroabsorption spectra of carotenoid cation radical and dication, S. Krawczyk 230 (1998) 297

-visible
Absorption and electroabsorption spectra of carotenoid cation radical and dication, S. Krawczyk 230 (1998) 297

Calorimetric methods
Dynamic heat capacity and reaction enthalpy during the two-stage network growth in diepoxide–diamine compositions, E. Tombari, C. Ferrari, G. Salvetti and G.P. Johari 230 (1998) 267

Photon counting and phase fluorimetry
Positronium states in the pores of silica gel, T. Goworek, K. Ciesielski, B. Jasińska and J. Wawryszczuk 230 (1998) 305

Electron impact spectroscopy
Valence orbital electron momentum distributions for oxygen: comparison of EMS measurements with theory, J. Rolke, Y. Zheng, C.E. Brion, Y.A. Wang and E.R. Davidson 230 (1998) 153

Laser induced fluorescence
Temperature effect on quenching of $CH(A^2\Delta)$, C. Chen, F. Wang, Y. Chen and X. Ma 230 (1998) 317

Ultrafast measurements
Higher excited-state photoisomerization and singlet to triplet intersystem-crossing in DODCI, S. Reindl and A. Penzkofer 230 (1998) 83

Nonlinear optics and spectroscopy
Higher excited-state photoisomerization and singlet to triplet intersystem-crossing in DODCI, S. Reindl and A. Penzkofer 230 (1998) 83
Numerical study of induced polarization dynamics in ultrafast spectral hole-burning experiments, R. Laenen and C. Rauscher 230 (1998) 223

Synchrotron spectroscopies
An experimental and theoretical study of the spectroscopic and thermodynamic properties of toluene, D.A. Shaw, D.M.P. Holland, M.A. MacDonald, M.A. Hayes, L.G. Shpinkova, E.E. Rennie, C.A.F. Johnson, J.E. Parker and W. von Niessen 230 (1998) 97

Coherent optical spectroscopy
Numerical study of induced polarization dynamics in ultrafast spectral hole-burning experiments, R. Laenen and C. Rauscher 230 (1998) 223

Atomic and molecular beam techniques
Nanosecond switching, field reversal evidence of Rydberg atom desorption from surfaces, L. Holmlid 230 (1998) 327

Mass spectroscopy
Projectile fragment–ion fragment–ion coincidences (PFIFICO) following fast ion impact on SF_6, M. Lange, O. Pfaff, U. Müller and R. Brenn 230 (1998) 117

Objects

Bulk systems

Gases
An ab initio study of electronic spectra and excited-state properties of 7-azaindole in vapour phase and aqueous solution, M.K. Shukla and P.C. Mishra 230 (1998) 187

Liquid mixtures and solutions
An ab initio study of electronic spectra and excited-state properties of 7-azaindole in vapour phase and aqueous solution, M.K. Shukla and P.C. Mishra 230 (1998) 187
Numerical study of induced polarization dynamics in ultrafast spectral hole-burning experiments, R. Laenen and C. Rauscher 230 (1998) 223

Glasses
Positronium states in the pores of silica gel, T. Goworek, K. Ciesielski, B. Jasińska and J. Wawryszczuk 230 (1998) 305

Polymers
Dynamic heat capacity and reaction enthalpy during the two-stage network growth in diepoxide–diamine compositions, E. Tombari, C. Ferrari, G. Salvetti and G.P. Johari 230 (1998) 267

Surfaces
A classical molecular dynamics study of the vibrational dynamics of the H/C(111)-(1 × 1) system, K.S. Smirnov, V.A. Ermoshin and D. Bougeard 230 (1998) 57
Theoretical approach of the infrared profile of molecular adsorbates on clean surfaces: inhomogeneous broadening, C. Girardet, J. Humbert and P.N.M. Hoang 230 (1998) 67
Nucleation in small capillary tubes, G.J. Brereton, R.J. Crilly and J.R. Spears 230 (1998) 253
Nanosecond switching, field reversal evidence of Rydberg atom desorption from surfaces, L. Holmlid 230 (1998) 327

Microscopic and mesoscopic systems

Single atoms, molecules and assemblies (incl. biological)
Theoretical study on the ionized states of ethylene by the SAC-CI (general-*R*) method, J. Hasegawa, M. Ehara and H. Nakatsuji 230 (1998) 23

Molecules (neutral and ionic)
Theoretical analysis of reactions related to the HNO_2 energy surface: OH + NO and H + NO_2, M.T. Nguyen, R. Sumathi, D. Sengupta and J. Peeters 230 (1998) 1
Projectile fragment–ion fragment–ion coincidences (PFIFICO) following fast ion impact on SF_6, M. Lange, O. Pfaff, U. Müller and R. Brenn 230 (1998) 117

An ab initio study of electronic spectra and excited-state properties of 7-azaindole in vapour phase and aqueous solution, M.K. Shukla and P.C. Mishra 230 (1998) 187
Theoretical study on the absorption spectra of pseudoisocyanine bromide (PIC-Br) molecular *J*-aggregates, T. Kato, F. Sasaki, S. Abe and S. Kobayashi 230 (1998) 209
Absorption and electroabsorption spectra of carotenoid cation radical and dication, S. Krawczyk 230 (1998) 297

-diatomic
On the electronic structure and spectroscopy of the ScN molecule, A. Daoudi, S. Elkhattabi, G. Berthier and J.P. Flament 230 (1998) 31
Valence orbital electron momentum distributions for oxygen: comparison of EMS measurements with theory, J. Rolke, Y. Zheng, C.E. Brion, Y.A. Wang and E.R. Davidson 230 (1998) 153

-small polyatomics
Theoretical study of structures, energetics and vibrational properties of BC_2H_3 species, N. Galland, Y. Hannachi, D.V. Lanzisera and L. Andrews 230 (1998) 143

-aromatics
Ab initio MO and density functional studies on the vibrational spectra of 1,4-benzoquinone, and its anion and dianion, C.-G. Zhan and S. Iwata 230 (1998) 45
Higher excited-state photoisomerization and singlet to triplet intersystem-crossing in DODCI, S. Reindl and A. Penzkofer 230 (1998) 83
An experimental and theoretical study of the spectroscopic and thermodynamic properties of toluene, D.A. Shaw, D.M.P. Holland, M.A. MacDonald, M.A. Hayes, L.G. Shpinkova, E.E. Rennie, C.A.F. Johnson, J.E. Parker and W. von Niessen 230 (1998) 97

-polymeric and biological
Dynamic heat capacity and reaction enthalpy during the two-stage network growth in diepoxide–diamine compositions, E. Tombari, C. Ferrari, G. Salvetti and G.P. Johari 230 (1998) 267
General treatment of vibrations of helical molecules and application to transition dipole coupling in amide I and amide II modes of α-helical poly(L-alanine), S.-H. Lee and S. Krimm 230 (1998) 277

Free radicals (incl. hydronium and muonium)
Study on the coherent spin motion of the radical-ion pair formed in the laser photolysis of *N,N,N′,N′*-tetramethyl-1,4-phenylenediamine in 2-propanol, Y. Iwasaki, H. Murai, K. Maeda and T. Azumi 230 (1998) 201
Temperature effect on quenching of $CH(A^2\Delta)$, C. Chen, F. Wang, Y. Chen and X. Ma 230 (1998) 317

Defects and impurities
Theoretical approach of the infrared profile of molecular adsorbates on clean surfaces: inhomogeneous broadening, C. Girardet, J. Humbert and P.N.M. Hoang 230 (1998) 67

Ions and charge carriers
Nanosecond switching, field reversal evidence of Rydberg atom desorption from surfaces, L. Holmlid 230 (1998) 327

Phenomena

Molecular structure

A quantum chemical ab initio study of the interaction between Co^+ and Ni^+ ions with CO_2 and N_2O, J.V. Burda 230 (1998) 13

On the electronic structure and spectroscopy of the ScN molecule, A. Daoudi, S. Elkhattabi, G. Berthier and J.P. Flament 230 (1998) 31

Ab initio MO and density functional studies on the vibrational spectra of 1,4-benzoquinone, and its anion and dianion, C.-G. Zhan and S. Iwata 230 (1998) 45

Theoretical study of structures, energetics and vibrational properties of BC_2H_3 species, N. Galland, Y. Hannachi, D.V. Lanzisera and L. Andrews 230 (1998) 143

Vibrations and rotations of molecules

On the electronic structure and spectroscopy of the ScN molecule, A. Daoudi, S. Elkhattabi, G. Berthier and J.P. Flament 230 (1998) 31

Ab initio MO and density functional studies on the vibrational spectra of 1,4-benzoquinone, and its anion and dianion, C.-G. Zhan and S. Iwata 230 (1998) 45

Theoretical study of structures, energetics and vibrational properties of BC_2H_3 species, N. Galland, Y. Hannachi, D.V. Lanzisera and L. Andrews 230 (1998) 143

General treatment of vibrations of helical molecules and application to transition dipole coupling in amide I and amide II modes of α-helical poly(L-alanine), S.-H. Lee and S. Krimm 230 (1998) 277

Surface chemical physics

-adsorption

Theoretical approach of the infrared profile of molecular adsorbates on clean surfaces: inhomogeneous broadening, C. Girardet, J. Humbert and P.N.M. Hoang 230 (1998) 67

-desorption

Nanosecond switching, field reversal evidence of Rydberg atom desorption from surfaces, L. Holmlid 230 (1998) 327

Electronic structure and states

A quantum chemical ab initio study of the interaction between Co^+ and Ni^+ ions with CO_2 and N_2O, J.V. Burda 230 (1998) 13

Theoretical study on the ionized states of ethylene by the SAC-CI (general-*R*) method, J. Hasegawa, M. Ehara and H. Nakatsuji 230 (1998) 23

On the electronic structure and spectroscopy of the ScN molecule, A. Daoudi, S. Elkhattabi, G. Berthier and J.P. Flament 230 (1998) 31

Valence orbital electron momentum distributions for oxygen: comparison of EMS measurements with theory, J. Rolke, Y. Zheng, C.E. Brion, Y.A. Wang and E.R. Davidson 230 (1998) 153

An ab initio study of electronic spectra and excited-state properties of 7-azaindole in vapour phase and aqueous solution, M.K. Shukla and P.C. Mishra 230 (1998) 187

Absorption and electroabsorption spectra of carotenoid cation radical and dication, S. Krawczyk 230 (1998) 297

Critical behavior and phase transitions
Nucleation in small capillary tubes, G.J. Brereton, R.J. Crilly and J.R. Spears 230 (1998) 253

Electric and magnetic properties
Absorption and electroabsorption spectra of carotenoid cation radical and dication, S. Krawczyk 230 (1998) 297

Spin splittings
Study on the coherent spin motion of the radical-ion pair formed in the laser photolysis of *N*,*N*,*N*′,*N*′-tetramethyl-1,4-phenylenediamine in 2-propanol, Y. Iwasaki, H. Murai, K. Maeda and T. Azumi 230 (1998) 201

Molecular interactions
Temperature effect on quenching of $CH(A^2\Delta)$, C. Chen, F. Wang, Y. Chen and X. Ma 230 (1998) 317

Spectral bandshapes and intensities
Theoretical approach of the infrared profile of molecular adsorbates on clean surfaces: inhomogeneous broadening, C. Girardet, J. Humbert and P.N.M. Hoang 230 (1998) 67

Molecular photophysical processes
Higher excited-state photoisomerization and singlet to triplet intersystem-crossing in DODCI, S. Reindl and A. Penzkofer 230 (1998) 83
An experimental and theoretical study of the spectroscopic and thermodynamic properties of toluene, D.A. Shaw, D.M.P. Holland, M.A. MacDonald, M.A. Hayes, L.G. Shpinkova, E.E. Rennie, C.A.F. Johnson, J.E. Parker and W. von Niessen 230 (1998) 97

Photochemistry
An experimental and theoretical study of the spectroscopic and thermodynamic properties of toluene, D.A. Shaw, D.M.P. Holland, M.A. MacDonald, M.A. Hayes, L.G. Shpinkova, E.E. Rennie, C.A.F. Johnson, J.E. Parker and W. von Niessen 230 (1998) 97

Intramolecular dynamics
Higher excited-state photoisomerization and singlet to triplet intersystem-crossing in DODCI, S. Reindl and A. Penzkofer 230 (1998) 83

-vibrational energy redistribution (incl. vibrational dissociation)
A classical molecular dynamics study of the vibrational dynamics of the H/C(111)-(1 × 1) system, K.S. Smirnov, V.A. Ermoshin and D. Bougeard 230 (1998) 57

Coherence loss processes
Study on the coherent spin motion of the radical-ion pair formed in the laser photolysis of *N*,*N*,*N*′,*N*′-tetramethyl-1,4-phenylenediamine in 2-propanol, Y. Iwasaki, H. Murai, K. Maeda and T. Azumi 230 (1998) 201

Nonlinear responses (incl. optical)
Numerical study of induced polarization dynamics in ultrafast spectral hole-burning experiments, R. Laenen and C. Rauscher 230 (1998) 223

Reactions (incl. dissociation)
Theoretical analysis of reactions related to the HNO_2 energy surface: OH + NO and H + NO_2, M.T. Nguyen, R. Sumathi, D. Sengupta and J. Peeters 230 (1998) 1
Semiclassical quantum unimolecular reaction rate theory revisited, S. Jang, M. Zhao and S.A. Rice 230 (1998) 237
Dynamic heat capacity and reaction enthalpy during the two-stage network growth in diepoxide–diamine compositions, E. Tombari, C. Ferrari, G. Salvetti and G.P. Johari 230 (1998) 267

-isolated molecules
An experimental and theoretical study of the spectroscopic and thermodynamic properties of toluene, D.A. Shaw, D.M.P. Holland, M.A. MacDonald, M.A. Hayes, L.G. Shpinkova, E.E. Rennie, C.A.F. Johnson, J.E. Parker and W. von Niessen 230 (1998) 97

-collisional
Projectile fragment–ion fragment–ion coincidences (PFIFICO) following fast ion impact on SF_6, M. Lange, O. Pfaff, U. Müller and R. Brenn 230 (1998) 117
Temperature effect on quenching of $CH(A^2\Delta)$, C. Chen, F. Wang, Y. Chen and X. Ma 230 (1998) 317

Positron annihilation
Positronium states in the pores of silica gel, T. Goworek, K. Ciesielski, B. Jasińska and J. Wawryszczuk 230 (1998) 305

Ionization (incl. Rydberg states)
Theoretical study on the ionized states of ethylene by the SAC-CI (general-*R*) method, J. Hasegawa, M. Ehara and H. Nakatsuji 230 (1998) 23
Nanosecond switching, field reversal evidence of Rydberg atom desorption from surfaces, L. Holmlid 230 (1998) 327